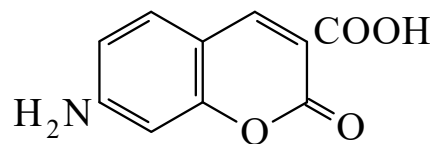




>>Entry Name: 7-Amino-2-oxo-2H-1-benzopyran-3-carboxylic acid

Synonym(s): 7-Aminocoumarin-3-carboxylic acid



CAS Registry Number: 100343-98-4

Molecular Formula: C₁₀H₇NO₄

Molecular Weight: 205.17

Accurate Mass: 205.037509

Percentage Composition: C 58.54%; H 3.44%; N 6.83%; O 31.19%

Physical Description: Orange cubes

Melting Point: Mp 233-235°. Mp 278°

>>Derivative: Me ester

Molecular Formula: C₁₁H₉NO₄

Molecular Weight: 219.196

Accurate Mass: 219.053159

Percentage Composition: C 60.28%; H 4.14%; N 6.39%; O 29.20%

Physical Description: Orange cubes

Melting Point: Mp 254°

>>Derivative: Et ester

CAS Registry Number: 72705-70-5

Molecular Formula: C₁₂H₁₁NO₄

Molecular Weight: 233.223

Accurate Mass: 233.068809

Percentage Composition: C 61.80%; H 4.75%; N 6.01%; O 27.44%

Physical Description: Cryst.

Melting Point: Mp 235.5°

>>Derivative: N-Ac

CAS Registry Number: 138196-52-8

Molecular Formula: C₁₂H₉NO₅

Molecular Weight: 247.207

Accurate Mass: 247.048074

Percentage Composition: C 58.30%; H 3.67%; N 5.67%; O 32.36%

Physical Description: Cryst.

Melting Point: Mp 280-282°. Mp 310-320°

>>Derivative: N,N-Di-Me, fluoride

Synonym(s): 7-(Dimethylamino)-2-oxo-2H-1-benzopyran-3-carbonyl fluoride, 9CI

CAS Registry Number: 132181-77-2

Molecular Formula: C₁₂H₁₀FNO₃

Molecular Weight: 235.214

Accurate Mass: 235.064472

Percentage Composition: C 61.28%; H 4.29%; F 8.08%; N 5.95%; O 20.41%

Use/Importance: Fluorescent derivatisation reagent for amines

Melting Point: Mp 233-235°

>>Derivative: N,N-Di-Et, hydrazide

Synonym(s): 7-(Diethylamino)-2-oxo-2H-1-benzopyran-3-carboxylic acid hydrazide, 9CI. 7-(Diethylamino)coumarin-3-carbohydrazide. Deccyl hydrazide. DCCH

Molecular Formula: C₁₄H₁₇N₃O₃

Molecular Weight: 275.307

Accurate Mass: 275.126992

Percentage Composition: C 61.08%; H 6.22%; N 15.26%; O 17.43%

Use/Importance: Used as derivatising agent for carboxylic acid detn., using peroxyoxalate chemiluminescence in liquid chromatography

References: